Benzoic acid, 4-hydroxy-3,5-dimethoxy-

Other names:	3,5-Dimethoxy-4-hydroxybenzoic acid
	3,5-Dimethoxy-4-hydroxybenzoic acid (syringic acid)
	4-Hydroxy-3,5-dimethylbenzoic acid
	4-hydroxy-3,5-dimethoxybenzoic acid
	Cedar acid
	syringic acid
Inchi:	InChI=1S/C9H10O5/c1-13-6-3-5(9(11)12)4-7(14-2)8(6)10/h3-4,10H,1-2H3,(H,11,12)
InchiKey:	JMSVCTWVEWCHDZ-UHFFFAOYSA-N
Formula:	C9H10O5
SMILES:	COc1cc(C(=O)O)cc(OC)c1O
Mol. weight [g/mol]:	198.17
CAS:	530-57-4

Physical Properties

Property code	Value	Unit	Source
gf	-512.31	kJ/mol	Joback Method
hf	-722.06	kJ/mol	Joback Method
hfus	26.18	kJ/mol	Joback Method
hvap	80.49	kJ/mol	Joback Method
log10ws	-1.32		Crippen Method
logp	1.108		Crippen Method
mcvol	138.960	ml/mol	McGowan Method
pc	4379.97	kPa	Joback Method
rinpol	1823.00		NIST Webbook
rinpol	1823.00		NIST Webbook
tb	713.47	K	Joback Method
tc	923.84	K	Joback Method
tf	485.80	K	Solubility and Thermodynamic Behavior of Syringic Acid in Eight Pure and Water + Methanol Mixed Solvents
vc	0.459	m3/kmol	Joback Method

Temperature Dependent Properties

Property code	Value	Unit	Temperature [K]	Source
cpg	412.86	J/mol×K	923.84	Joback Method
cpg	406.19	J/mol×K	888.78	Joback Method
cpg	399.15	J/mol×K	853.72	Joback Method
cpg	391.71	J/mol×K	818.66	Joback Method
cpg	383.84	J/mol×K	783.59	Joback Method
cpg	375.52	J/mol×K	748.53	Joback Method
cpg	366.72	J/mol×K	713.47	Joback Method
dvisc	0.0001015	Pa×s	509.58	Joback Method
dvisc	0.0000039	Pa×s	713.47	Joback Method
dvisc	0.0000059	Pa×s	679.49	Joback Method
dvisc	0.0000092	Pa×s	645.51	Joback Method
dvisc	0.0000152	Pa×s	611.53	Joback Method
dvisc	0.0000265	Pa×s	577.54	Joback Method
dvisc	0.0000498	Pa×s	543.56	Joback Method
hfust	33.70	kJ/mol	480.30	NIST Webbook

Sources

Crippen Method: https://www.chemeo.com/doc/models/crippen_log10ws

Crippen Method: **Solubility of some phenolic compounds in aqueous alkali metal nitrate solutions from (293.15 to 318.15) K:** https://www.doi.org/10.1016/j.jct.2008.06.006

Temperature and salt addition effects on the solubility behaviour of some phenolic compounds in water: http://pubs.acs.org/doi/abs/10.1021/ci990307l

Solubility of Syringic and Vanillic Acids in Supercritical Carbon Dioxide: https://www.doi.org/10.1016/j.jct.2006.06.014

McGowan Method: https://www.doi.org/10.1021/je034129a

NIST Webbook: http://link.springer.com/article/10.1007/BF02311772

Solubility of Gallic Acid, Vanillin, Syringic Acid, and Protocatechuic Acid in Aqueous Sulfate Solutions from (293.15 to 318.15) K: http://webbook.nist.gov/cgi/cbook.cgi?ID=C530574&Units=SI

Joback Method: https://www.doi.org/10.1021/je800205e

Solubility and Thermodynamic Behavior of Syringic Acid in Eight Pure and Water + Methanol Mixed Solvents: https://en.wikipedia.org/wiki/Joback_method

https://www.doi.org/10.1021/acs.jced.7b00333

Legend

cpg: Ideal gas heat capacity

dvisc: Dynamic viscosity

gf:	Standard Gibbs free energy of formation
hf:	Enthalpy of formation at standard conditions
hfus:	Enthalpy of fusion at standard conditions
hfust:	Enthalpy of fusion at a given temperature
hvap:	Enthalpy of vaporization at standard conditions
log10ws:	Log10 of Water solubility in mol/l
logp:	Octanol/Water partition coefficient
mcvol:	McGowan's characteristic volume
pc:	Critical Pressure
rinpol:	Non-polar retention indices
tb:	Normal Boiling Point Temperature
tc:	Critical Temperature
tf:	Normal melting (fusion) point
vc:	Critical Volume